

Landauer-like formula for dissipative tunneling

S.G. Chung

Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Str. 38, D-01187 Dresden, Germany

The Landauer formula for electrical conductance is simple but works remarkably well in mesoscopic systems. We propose a Landauer-like formula for calculating an escape rate out of a dissipative metastable well, the quantum Kramers rate. The proposed formula works well in the current-voltage characteristic of a single Josephson junction.

05.40.-a, 05.60.-k, 73.40.Gk, 74.50.+r

The electrical conduction is a typical non-equilibrium phenomenon. Two theories are known. One is the Green-Kubo-Nakano linear response theory [1] and the other is the Landauer theory [2]. The former has a generality but often technically challenging. The latter, on the other hand, lacks a generality and limited to mesoscopic systems so far such as quantum wires, but is intuitive, simple and practically quite useful.

The system Landauer considered is composed of a sample which is connected by two leads to the electron reservoirs with chemical potentials $\mu_{1,2}$. The voltage applied is $V = -(\mu_1 - \mu_2)/e$. The electrons which contribute to the net current are those electrons with energies between μ_1 and μ_2 . Write the energy of electrons with wave number k as $E(k)$, then it contributes $-e(dE/\hbar dk)T(k)$ where $T(k)$ denotes the transmission rate. Assuming that any electron supply and removal from reservoirs are immediate, the net current is simply, including factor 2 for up and down spins,

$$I = -2e \int_{k_1}^{k_2} \frac{dk}{2\pi} \frac{dE}{\hbar dk} T(k) \quad (1)$$

where $\mu_{1,2} = E(k_{1,2})$. When $\mu_1 \sim \mu_2$ and $T(k) = \text{const} = T$, one gets the conductance

$$G = \frac{I}{V} = \frac{2e^2}{h} T \quad (2)$$

The purpose of the present paper is to propose a Landauer-like formula for calculating a particle's escape rate out of a dissipative metastable well, the so-called quantum Kramers rate. This well-defined and universal problem is ubiquitous in quite a wide range of physics and attracted much attention over decades [3–7]. The latest review article discussed a seemingly ultimate issue of full dynamical analysis in the presence of time-dependent external driving force [6]. In spite of all these quite intensive studies, however, the issue appears to be still open. The situation looks somehow similar to the problem of electrical conductance. As mentioned above, we have the linear response theory which is exact but often technically challenging and the Landauer theory which is limited but intuitive, simple and has seen a remarkable success in mesoscopic systems. It may be worth

pursuing an analogous simple formula for the quantum Kramers rate.

First note that (1) is a sum of individual contributions $(dE/\hbar dk)T(k)$ which is nothing but a right going flux. A corresponding quantity in the escape rate is the probability of finding particle moving rightward at the top of the potential barrier. Adding all such contributions, we might reach a formula

$$v_{qts} = \text{Tr} [e^{-\beta H} \mathcal{F} \Theta(p)] / Z_0 \equiv \frac{1}{2M} \langle \delta(x) | p | \rangle \quad (3)$$

where Z_0 is the partition function of the metastable well, $\mathcal{F} \equiv \delta(x)p/M$ with $p = -i\hbar\partial_x$ is the flux at the barrier top and $\Theta(p)$ is the unit step function. The formula (3) is nothing but the quantum transient state (QTS) theory long known in chemistry for calculating molecular reaction rates [8]. Historically, the QTS theory first appeared as an approximation to a formally exact expression from scattering theory [9],

$$v_{exact} = \text{Re} \langle \mathcal{F} \mathcal{P} \rangle \quad (4)$$

where Re means to take the real part and the operator

$$\mathcal{P} = \lim_{t \rightarrow \infty} e^{iHt/\hbar} \Theta(p) e^{-iHt/\hbar} \quad (5)$$

projects onto all states that have positive momentum in the infinite future. The exact expression (4) can be manipulated to give [9]

$$v_{exact} = \frac{1}{2} \int_{-\infty}^{\infty} dt \langle \mathcal{F}(0) \mathcal{F}(t) \rangle \quad (6)$$

where $\mathcal{F}(t)$ is the Heisenberg picture of the operator \mathcal{F} .

The formula (6) takes precisely the form of the Green-Kubo-Nakano formula for the electrical conductance. The QTS theory was obtained from the exact one (4) by simply replacing $\mathcal{P} \rightarrow \Theta(p)$ thereby neglecting all the dynamical processes. The QTS formula (3), however, is not well-defined quantum mechanically because the operator \mathcal{F} is ambiguous. The necessary regularization of such operators as \mathcal{F} is done by the Weyl rule [5]. Let us write (3) as

$$v_{qts} = \frac{1}{2MZ_0} \int \int dx dx' \times \langle x | e^{-\beta H} | x' \rangle \langle x' | \delta(x) | p | | x \rangle \quad (7)$$

Now the Weyle rule gives a quantum operator from a classical one, $\mathcal{F}_{cl}(p, q) \rightarrow \mathcal{F}_{op}(p, q)$, in coordinate matrix representation [8],

$$\langle x' | \mathcal{F}_{op} | x \rangle = \frac{1}{h} \int dp e^{-ip(x-x')/\hbar} \mathcal{F}_{cl} \left(p, \frac{x+x'}{2} \right) \quad (8)$$

Applied to the last term in (7), we have

$$\begin{aligned} \langle x' | \delta(x) | p | x \rangle &= \frac{1}{h} \int dp e^{-ip(x-x')/\hbar} |p| \delta \left(\frac{x+x'}{2} \right) \\ &= \frac{\hbar}{\pi} \delta \left(\frac{x+x'}{2} \right) \partial_x \left(\frac{1}{x-x'} \right) \end{aligned} \quad (9)$$

Putting (9) into (7) and integrating in parts gives

$$v_{qts} = \frac{\hbar}{4\pi M Z_0} \int dx \left(-\frac{1}{x} \right) \partial_x \langle x | e^{-\beta H} | -x \rangle \quad (10)$$

Some comments are due on the Weyle rule. First, it is not exact. For example, if one proceeds with this rule for the propagator $e^{-iHt/\hbar}$ with $H = p^2/2M + V(x)$, the Weyle rule gives only a *short time approximation* [10]. In general, as one can easily see from (8), the more complicated the functional forms of coordinate and momentum, unless they are functions of coordinate alone or momentum alone, the more dubious results are obtained by the Weyle rule. Back to the propagator, because it is already Hermite, the classical and quantum expression take the same form. Thus the failure of the Weyle rule resides in an inability of doing proper commutation calculations for complicated mixtures of coordinate and momentum. In fact when the starting classical form is simple enough, e.g. xp , then the Weyle rule is known to give a correct answer, e.g. $(xp + px)/2$. It is certainly embarrassing that we still do not know how to construct correct quantum mechanical operators from classical quantities when they are complicated enough. Second, a connection to the more familiar Wigner distribution function should be mentioned. In fact we have for any operator \mathcal{O} ,

$$\langle \mathcal{O} \rangle = \iint dx dx' \langle x | e^{-\beta H} | x' \rangle \langle x' | \mathcal{O}_{op} | x \rangle \quad (11)$$

Using the Weyle rule (8) for the last term in (11) and changing the variables as $x - x' = r$, $\frac{x+x'}{2} = q$, we have

$$\langle \mathcal{O} \rangle = \iint dp dq \mathcal{O}_{cl}(p, q) W(p, q) \quad (12)$$

where the Wigner distribution function $W(p, q)$ is the Wigner representation of the density matrix [5],

$$W(p, q) \equiv \frac{1}{h} \int dr e^{-ipr/\hbar} \langle q + \frac{r}{2} | e^{-\beta H} | q - \frac{r}{2} \rangle \quad (13)$$

The expression (12) *should not* be confused with the formally exact expression

$$\langle \mathcal{O} \rangle = \iint dp dq \mathcal{O}_W(p, q) W(p, q) \quad (14)$$

where \mathcal{O}_W is the Wigner representation of the operator \mathcal{O} ,

$$\mathcal{O}_W = \int dr e^{-ipr/\hbar} \langle q + \frac{r}{2} | \mathcal{O}_{op} | q - \frac{r}{2} \rangle \quad (15)$$

It is a simple exercise to check that \mathcal{O}_W reduces to \mathcal{O}_{cl} if the term in (15) is *approximated* by the Weyle rule (8). Third, as is seen in (9) and (10), the term $\delta(q) = \delta(\frac{x+x'}{2})$ results in an antiperiodic paths $\langle x | e^{-\beta H} | -x \rangle$ in the expression (10). The nonlocality, an integral over x rather than just a contribution at the barrier top $x = 0$, however, arises from the step function $\Theta(p)$. It is noted that some nonlocal contribution is certainly negative reflecting the fact that the Wigner distribution function is a quasi-probability function. It is also noted that the nonlocality does not show up when the QTS formula is treated by a semiclassical approximation (see e.g. Eq(2.22) in the second paper in [8]).

We have critically reviewed the QTS theory (10) as a candidate for the Landauer-like formula for the quantum Kramers rate. Two major approximations involved are (A) static or transient-state approximation and (B) the Weyle rule (8). The step function $\Theta(p)$ or equivalently $|p|$ under the trace operation is found to be a *dangerous* operator for the Weyle procedure, leading to nonlocality and associated possible negativity. Our idea in this paper is to get rid of this dangerous operator by taking *square* and *square root*. We thus propose a Landauer-like formula

$$v_{Li} = \frac{1}{2M} \sqrt{\langle \delta(x) p^2 \rangle / L} \quad (16)$$

where L is the size of the potential well. The factor L and the square root operation arises dimensionally and the fact that \mathcal{F} is a density operator containing $\delta(x)$. The proposed formula also makes the Kramers rate calculable from the *local*, at the barrier top, particle state. The factor $1/2$ takes into account only half of the contribution, outgoing one. It may be worth emphasizing that the p^2 operator rather than $\Theta(p)$ or $|p|$ would make the Weyle rule less dubious. Now, proceeding as before, we have

$$v_{Li} = \frac{\hbar}{2M} \sqrt{-\frac{1}{4LZ_0} \partial_x^2 \langle x | e^{-\beta H} | -x \rangle |_{x=0}} \quad (17)$$

which should be compared with the QTS formula (10).

Note that the proposed formula (17), unlike the QTS formula (10), is manifest local. In fact the difference between the QTS formula and the proposed one resides in a quantum fluctuation. To see this, consider

$$\begin{aligned} \langle \delta(x) | p | \rangle^2 &= \sum_{n, n'} \langle n | e^{-\beta H} \delta(x) | p | \\ &\times \left[\frac{|n \rangle \langle n'| e^{-\beta H} \delta(x)}{Z_0} \right] | p | | n' \rangle / Z_0 \end{aligned}$$

where the plane wave complete set may be used for $\{n\}$. Neglecting a quantum fluctuation, the term $[\dots] \rightarrow \delta_{n n'} < n|\delta(x)|n' >$, we reach

$$< \delta(x)|p| >^2 \longrightarrow < \delta(x)p^2 > / L \quad (18)$$

We have tested the proposed formula (16) versus the QTS formula (3) for the $I - V$ characteristic of the single Josephson junction (JJ). The resistively shunted and current biased single JJ is described by the action for the superconducting phase difference between the two superconductors [11],

$$S = \int_0^{\beta\hbar} d\tau \left[\frac{C}{2} \left(\frac{\hbar}{2e} \dot{\phi} \right)^2 + U(\phi) \right] - \int_0^{\beta\hbar} \int_0^{\beta\hbar} d\tau d\tau' \alpha(\tau - \tau') \cos \left(\frac{\phi(\tau) - \phi(\tau')}{2} \right)$$

$$U(\phi) = -E_J \cos \phi - \frac{I\hbar}{2e} \phi$$

$$\alpha(\tau) = \frac{\hbar}{2\pi e^2 R_T} \frac{(\pi/\beta\hbar)^2}{\sin^2(\pi\tau/\beta\hbar)} \quad (19)$$

where C is the capacitance, R_T the shunt resistance, I the bias current and E_J the Josephson energy. Thermal over-the-hill motion or quantum tunneling of the phase gives rise to a voltage $V = \hbar\dot{\phi}/2e$ (the Josephson relation) with $\dot{\phi} = [\phi, H]/i\hbar = (2e)^2 n / \hbar C$ where $n = -i\partial_\phi$ is the number of the Cooper pairs. So the flux operator here is

$$\mathcal{F} = \delta(\phi - \phi_0) \frac{(2e)^2}{\hbar C} n \quad (20)$$

where ϕ_0 denotes a maximum point of the potential $U(\phi)$. Taking into account the backward flux by a detailed balance, we have

$$\frac{V}{e/2C} = [1 - \exp(-\pi I\hbar\beta/e)] \times \frac{1}{2} \sqrt{\langle \delta(\phi - \phi_0)n^2/L \rangle} \quad (21)$$

After some manipulations, one can express the average in (21) as

$$\langle \delta(\phi - \phi_0)n^2 \rangle = Z/Z_0$$

$$Z = -\frac{1}{4} \partial_\phi^2 W(\phi, 2\phi_0 - \phi)|_{\phi = \phi_0}$$

$$Z_0 = \int d\phi W(\phi, \phi)$$

$$W(\phi, \phi') = \int_{\phi \rightarrow \phi'} \mathcal{D}\tilde{\phi} \exp(-S/\hbar) \quad (22)$$

where $\tilde{\phi}(0) = \phi$ and $\tilde{\phi}(\beta\hbar) = \phi'$.

The path-integral (22) with the action S given by (19) can be evaluated precisely by the cluster transfer matrix (CTM) method [12]. In the present problem, however, the dimensionless junction conductance $g \equiv R_q/R_T$

where $R_Q = h/4e^2 = 6.45 K\Omega$ is the quantum resistance, is at $g \lesssim 1$, and from the study of the single electron box which has a similar action as (19), this regime of g can be accurately handled by the 1-cluster TM method [13].

For a fixed g , the temperature dependence of the resistance changes from insulator-like behavior $\frac{dR}{dT} < 0$ to superconductor-like $\frac{dR}{dT} > 0$ with increasing ratio E_J/E_C where $E_C \equiv \frac{e^2}{2C}$. Repeating the calculations for different g , we can thus map a superconductor-insulator (SI) phase diagram in the $E_J/E_C - g$ plane. Fig. 1 shows a SI phase diagram at $T=80$ mK. The corresponding experimental results are denoted by open circles (S-like) and solid circles (I-like) [14,15]. Our result is the open diamond, the band-theory result the thick solid line [16], and the QTS result is denoted by triangles. While there is an issue of temperature dependence concerning the phase diagram [13], the agreement between the previous theory and experiments with the proposed method, not with the QTS theory, will be evident. A major disagreement between theory and experiment is for some data points near $g = 2.8$ [15]. However a similar phase diagram experimentally found for the 2D JJ arrays with similar parameter ranges for $g, E_J/E_C$ and T is bounded, $E_J/E_C \lesssim 0.5$, and $g \lesssim 0.5$ (cf. Fig 3 in [17]). The above data near $g = 2.8$ is currently mysterious.

In conclusion, we have proposed a new formula for calculating the quantum Kramers rate which may correspond to the Landauer formula for electrical conductance. The single Josephson junction for which the proposed formula was tested is quite general: It contains quantum fluctuation, dissipation and external bias. The reasonable outcome of the proposed formula in comparison with experiments and the previous theory, although the latter is not free from criticism [13], may be encouraging a further testing of the proposed method in a variety of physical systems. On the other hand, we must also admit that the new formula was derived in an attempt for technical improvement over the QTS theory. A contemplation of deep physical argument leading directly to the proposed formula is much desired.

This work was supported by the Visitor Program of the MPI-PKS. The work was also partially supported by the NSF under Grant No. DMR990002N and utilized the SGI/CRAY Origin2000 at the National Center for Supercomputing Applications at the University of Illinois at Urbana-Champaign. I thank Yoshiro Kakehashi, Mitsuhiro Arikawa and Klaus Morawetz for helpful discussions and bringing important references to my attention. I also thank Peter Hänggi and Anthony Leggett for enlightening conversations.

- [1] R. Kubo, J. Phys. Soc. Japan **12**, 570(1957).
- [2] R. Landauer, IBM J. Res. & Dev. **1**, 223(1957).
- [3] P. Hänggi, P. Talkner and M. Borkovec, Rev. Mod. Phys. **62**, 251(1990).
- [4] V.I. Mel'nikov, Phys. Rep. **209**, 1(1991)
- [5] U. Weiss, *Quantum Dissipative Systems*, 2-nd ed., Series in Modern Condensed Matter Physics, Vol. 10 (World Scientific, Singapore, 1998).
- [6] M. Thorwart, M. Grifoni and P. Hänggi, cond-mat/0102038.
- [7] T. Dittrich, P. Hänggi, G.-L. Ingold, B. Kramer, G. Schön and W. Zwerger, *Quantum Transport and Dissipation* (Wiley-VCH Verlag, 1998).
- [8] W.H. Miller, J. Chem. Phys. **61**, 1823(1974); **62**, 1899(1975).
- [9] T. Yamamoto, J. Chem. Phys., **33**, 281(1960); W.H. Miller, S.D. Schwartz and J.W. Tromp, *ibid.* **79**, 4889(1983).
- [10] R.P. Feynman and A.R. Hibbs, *Quantum Mechanics and Path Integrals* (McGraw-Hill, New York, 1965).
- [11] U. Eckern, G. Schön, and V. Ambegaokar, Phys. Rev. B **30**, 6419(1984)
- [12] S.G. Chung, J. Korea Phys. Soc. **33**, S25(1998); J. Phys. Soc. Japan **68**, 1778(1999).
- [13] S.G. Chung, unpublished.
- [14] J.S. Penttilä, Ü. Parts, P.J. Hakonen, M.A. Paalanen and E.B. Sonin, Phys. Rev. Lett. **82**, 1004(1999).
- [15] R. Yagi, S. Kobayashi and Y. Otuka, J. Phys. Soc. Japan **66**, 3722(1997).
- [16] K.K. Likharev and A.B. Zorin, J. Low Temp. Phys. **59**,

347(1985).

- [17] T. Yamaguchi, R. Yagi, A. Kanda, Y. Ootuka and S. Kobayashi, Phys. Rev. Lett. **85**, 1974(2000).

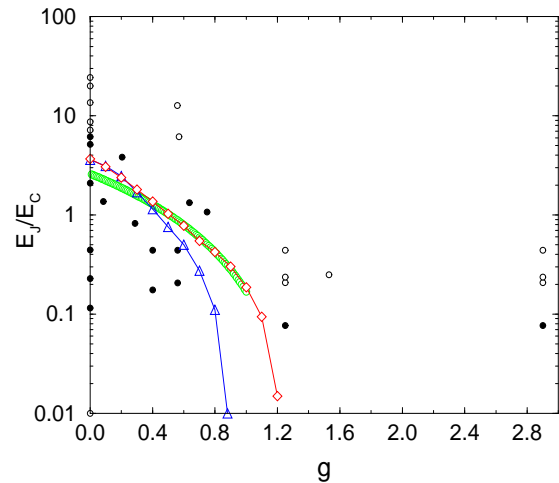


FIG. 1. Phase diagram of the single Josephson junction. The phase boundary lies between the insulator-like (solid circles) and superconductor-like (open circles) samples experimentally found in [14,15]. The thick line is the band theory [16] at $T = 80$ mK. The triangle is the QTS theory and diamond is due to the present theory at $T = 80$ mK.